FASTMath Tech Area Summary: Time Integrators

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The time integrator area is developing time integration methods and software for use in SciDAC applications

Includes two major efforts:

- Multirate methods in the Suite of Nonlinear and Differential-Algebraic Solvers (SUNDIALS)
  - Developing new methods and utilizing some developed in the base program work by Sandu et al.
- Parallel-in-time methods in SUNDIALS utilizing the XBraid software
  - XBraid supported by base program

Synergistic activities between time integration and other FASTMath:

- Spectral deferred correction methods and software for structured grids (in AMReX)
  - New methods planned for AMReX may include hybrid SDC-exponential integrators being developed in base program
- Multirate methods for structured grid systems (SUNDIALS with AMReX)
- Time integrators with adjoint sensitivities for optimization (PETSc)
  - Utilized by MMiCCS center and base program projects

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The time integrator team and its synergistic activities span three laboratories and one university

LLNL: Carol Woodward, David Gardner, and John Loffeld

Southern Methodist University: Daniel Reynolds

LBNL: Michael Minion

ANL: Hong Zhang, Barry Smith, Alp Dener

SciDAC application interactions

- (BER) Assessing and Improving the Numerical Solution of Atmospheric Physics in E3SM, PI: Hui Wan (PNNL)
  - Assessing time integration convergence in E3SM climate physics and improving time integration accuracy/stability

- (FES) Partnership for Multiscale Gyrokinetic Turbulence, PI: David Hatch (UT Austin) – See Darin Ernst's talk
  - Interfacing IMEX and multirate methods from SUNDIALS ARKode in 2D test code
  - Interfacing KINSOL nonlinear solver from SUNDIALS to provide acceleration for fixed point solve in Tango code

- (BER) A Non-hydrostatic Variable Resolution Atmospheric Model in ACME, PI: Mark Taylor (SNL)
  - Used ARKode in new E3SM nonhydrostatic dynamical core to test over 100 integration approaches and determine most efficient
  - Ongoing support of ARKode use in E3SM

Through FASTMath we are developing high order multirate time integrators in SUNDIALS

- Applications will become more multiphysics and multirate as they take advantage of exascale systems
- Many commonly used splitting schemes can suffer from low accuracy and/or poor/unknown stability
- Greater flexibility in time integration libraries is needed to meet the needs of multiphysics applications
- We are expanding the capabilities of the SUNDIALS ARKode package to meet these needs
  - Adding adaptive step multirate integration methods

$$y' = f_{\text{fast}}(y) + f_{slow}(y)$$

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We restructured the SUNDIALS ARKode package to provide infrastructure for general, adaptive, one-step methods

- ARKode provides the outer time integration loop and generic usage modes
- Time-stepping modules handle problem-specific components

Released modules:

- *ARKStep* – single-rate explicit, implicit, and IMEX RK methods
- *ERKStep* – a streamlined module for explicit methods
- *MRIStep* – module for multirate infinitesimal step methods
  - SUNDIALS 4.0: ARKode MRIStep module supporting explicit/explicit 2nd and 3rd order MIS methods.
  - SUNDIALS 5.0-dev.0: Support for implicit and IMEX fast methods and adaptive fast time steps in MRIStep

In development: *IMEXGARKStep* – module for IMEX Generalized Additive Runge-Kutta

See poster by David Gardner

1D Advection with Brusselator Reactions

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + k_1 A - k_2 B u + k_3 u^2 v - k_4 u$$
$$\frac{\partial v}{\partial t} = -c\frac{\partial v}{\partial x} + k_2 B u - k_3 u^2 v$$

- Compare 3rd order IMEX and MIS (multirate) methods
- Explicit (slow) advection and implicit (fast) reactions

	IMEX	MRI
Steps	6,805	1,429 / 8,813
Advection evals	29,379	4,288
Reaction evals	98,917	116,949

Same solution quality with 85% fewer advection evaluations (reduces parallel communication)

- Gains with MRI depend on the separation of time scales e.g., CFL vs reaction rates.

See poster by David Gardner

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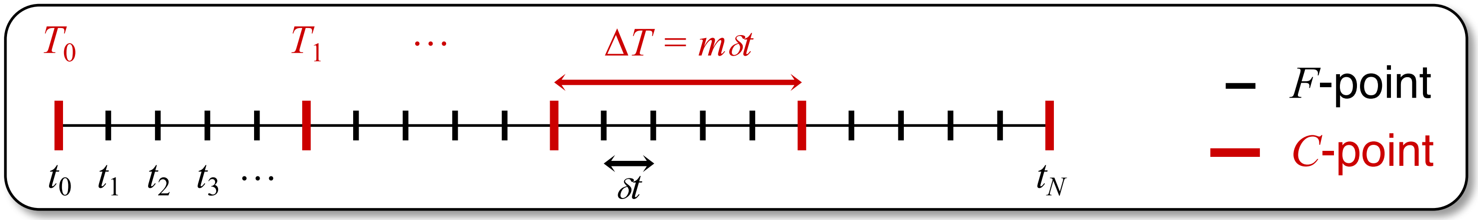
We will be adding a parallel-in-time capability to SUNDIALS through multigrid reduction in time (MGRIT)

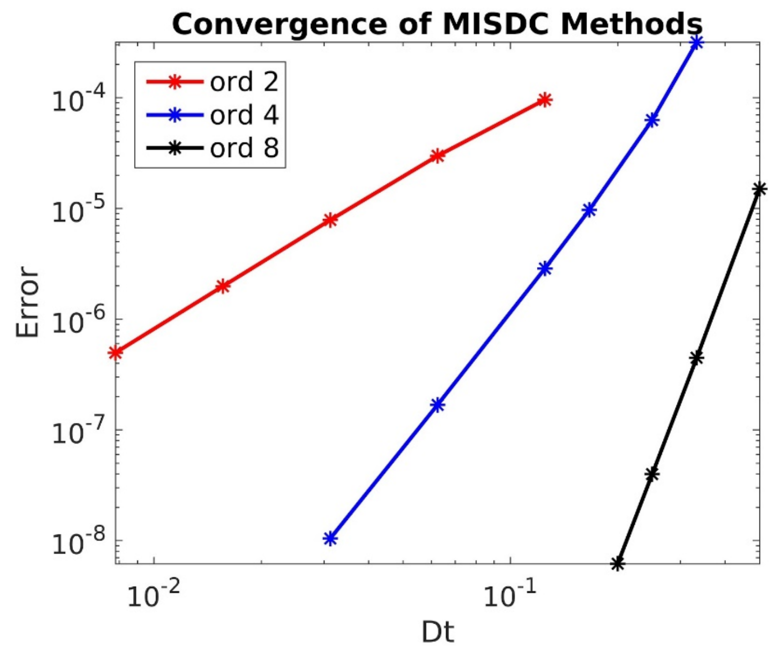
- MGRIT uses multiple coarse grids to update the fine grid solution



- Addressing challenges associated with multistep methods and use of variable step adaptive methods
- Initial work (through Off. Electricity project) shows parallel speedups with multi-stage and multistep adaptive step methods
- In year 3 we will connect the LLNL XBraid package with SUNDIALS to deliver MGRIT capability

General support for spectral deferred corrections integration enabled in AMReX structured adaptive mesh framework

- Large-scale computing platforms allow for highly complex multiphysics simulations, but these systems are often integrated with low-order splittings
  - SDC provides high-order time integration through iterations over the native operator split solution procedure
  - Prior support for SDC was specific to certain applications
  - Code and tutorial included in AMReX repo
  - FY18 work provided the capability to allow straightforward construction of high-order semi-implicit and multi-implicit integrators for problems with one or more stiff terms
  - FY19 work extends SDC to multirate integration for AMR



High-order convergence of a multi-implicit SDC integrator run on a 2D advection-diffusion-reaction system

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We are collaborating with the structured mesh team to investigate three-rate IMEX methods for AMR grids

- Working with the AMReX team, we are developing multirate methods for advection-diffusion-reaction systems

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = f_a(y_1) + f_d(y_1) + f_r(y_2)$$

- Methods will include both implicit and explicit algorithms

- Implementation will be in ARKode and tested through an interface within AMReX

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We have enabled some multirate time stepping of AMReX problems using SUNDIALS

Currently parallel single-level and multi-level time stepping if Δt is the same on all levels:

- SUNDIALS wrap of AMReX vector structure
- IMEX, or implicit stepping if the implicit portion is in the form $(\alpha A - \beta \nabla \cdot B \nabla)\phi = f$
  - Wrap of AMReX La Placian linear solver as a SUNDIALS linear solver package
  - Two-rate implicit-fast methods implemented. Implicit-slow methods in progress
- Demonstrated via multirate stepping of single- and multi-level Gray-Scott (two-rate) reaction-diffusion problem

See poster by John Loffeld

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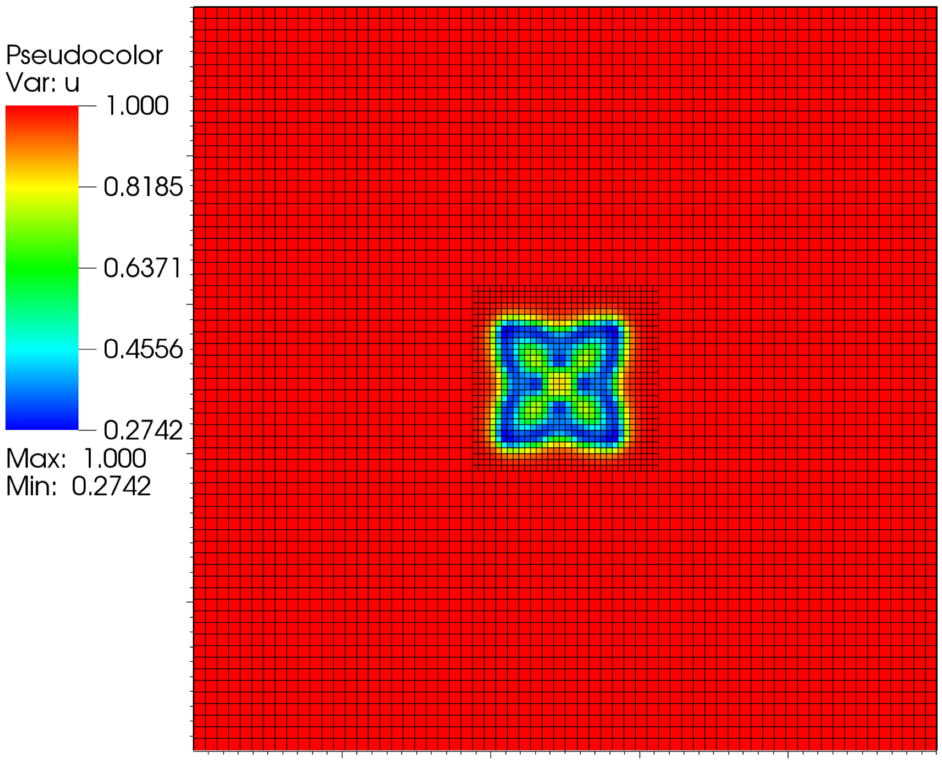
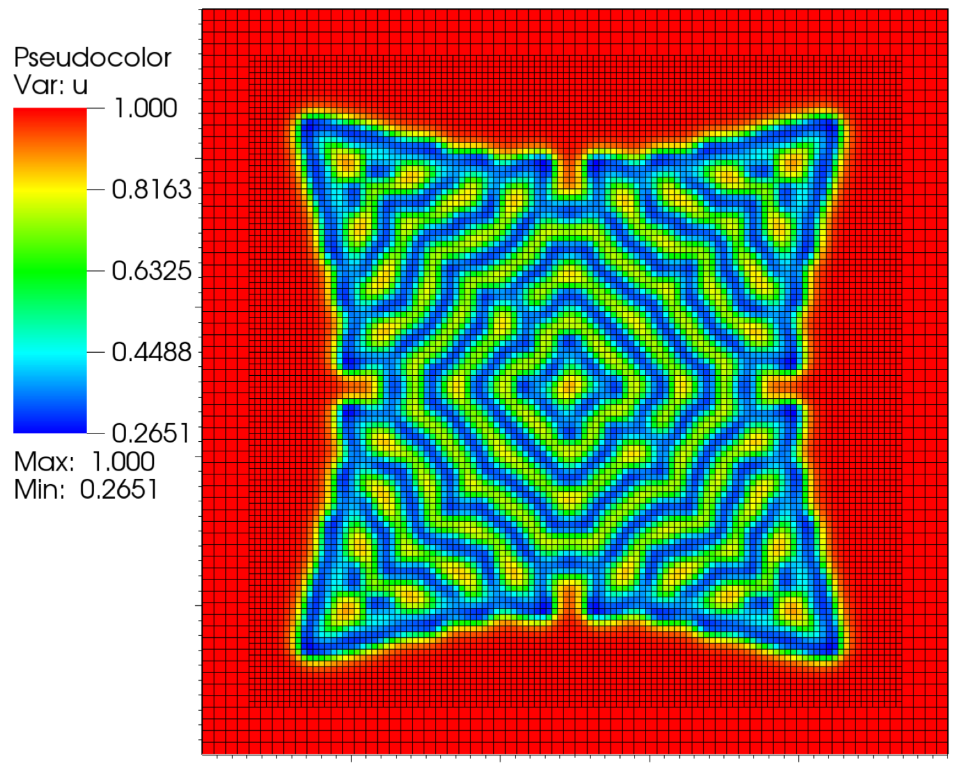
Gray-Scott equation computed with third-order explicit-explicit MIS multirate method

$$\frac{\partial u}{\partial t} = A\nabla^2 u - uv^2 + f(1-u), \quad \frac{\partial v}{\partial t} = B\nabla^2 v + uv^2 - (f+k)v$$



t = 1000

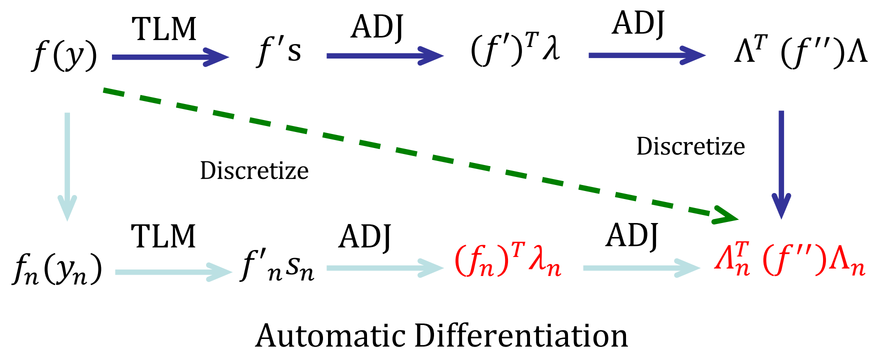


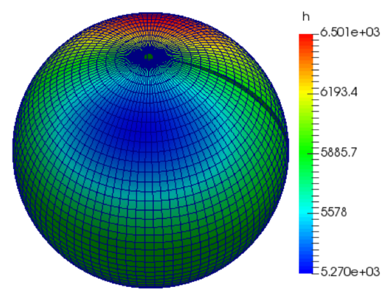
t = 5000

See poster by John Loffeld

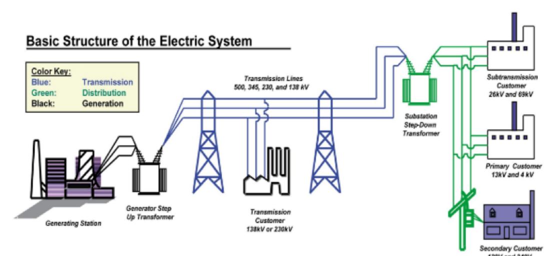
Sensitivity analysis integrator tools for PDE-constrained optimization

- **New composable and scalable discrete-adjoint solvers in PETSc for local sensitivity analysis**
  - Used discretize-then-differentiate approach, overcomes difficulties with Automatic Differentiation
  - Optimal adjoint checkpointing utilizes hierarchical memory
  - Implementation allows multiple objective functions and time intervals
- **Efficient gradients and Hessian-vec products for PDE-constrained opt**
  - Applications in climate data assimilation and power grid
  - New 2nd-order adjoints accelerate convergence of optimization algs





Adjoint-based 4D-Var global data assimilation



Optimal economic dispatch for dynamic power system

See poster by Hong Zhang

S. Abhyankar, J. Brown, E. Constantinescu, D. Ghosh, B. Smith, H. Zhang, PETSc/TS: A Modern Scalable ODE/DAE Solver Library, arXiv:1806.01437

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Our work in ECP provides greater capabilities for SciDAC applications

- SUNDIALS project in ECP
  - Redesign of nonlinear and linear solver interfaces
  - Encapsulation of nonlinear solvers
  - Addition of many-vector interface

- Participating in math libraries software development kit, PI: Yang; developing interoperability layers with SuperLU_DIST, PETSc, *hypre*, AMReX, MFEM, etc.

- Working with AMReX team to optimize use of SUNDIALS for reaction systems on GPUs

FASTMath integrators are used in numerous non-SciDAC DOE applications

- (OE) Supporting use of the IDA DAE integrator in the development of the GridDyn time domain power grid simulation package, PI: Philip Top (LLNL)
- (BER) Supporting use of KINSOL nonlinear solvers in the ParFlow watershed simulation package, PI: Reed Maxwell (CO School of Mines)
- (FES) BOUT++ fusion code uses CVODE as its time integrator
- (ECP) Supporting use of CVODE as an option in AMReX as a reaction integrator; through AMReX have impact on the Nyx cosmology code
- (ECP) CVODE used in the NEK5000 code for reactor modeling
- Numerous other applications throughout DOE and worldwide

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